(FILE 'HOME' ENTERED AT 17:56:05 ON 28 SEP 2003)

FILE 'REGISTRY' ENTERED AT 17:56:19 ON 28 SEP 2003
L1 STRUCTURE UPLOADED
L2 0 S L1
L3 48 S L1 FUL
L4 0 S BENZAL/CN

FILE 'REGISTRY' ENTERED AT 17:57:49 ON 28 SEP 2003
L5 0 S BENZAL/CN
L6 1 S BENZAL BROMIDE/CN
L7 1 S BROMINE/CN

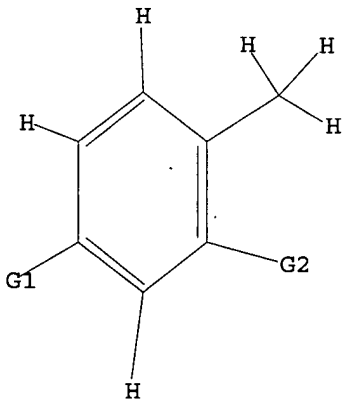
FILE 'CAPLUS, USPATFULL' ENTERED AT 17:59:20 ON 28 SEP 2003
L8 38 S L3
L9 146 S L6
L10 31230 S L7
L11 0 S L8 AND L9
L12 0 S L8 AND L10

FILE 'REGISTRY' ENTERED AT 18:02:03 ON 28 SEP 2003
L13 STRUCTURE UPLOADED
L14 1 S L13
L15 12 S L13 FUL

FILE 'CAPLUS, USPATFULL' ENTERED AT 18:02:50 ON 28 SEP 2003
L16 2321 S L15
L17 2 S L8 AND L16

FILE 'CASREACT' ENTERED AT 18:08:05 ON 28 SEP 2003
L18 STRUCTURE UPLOADED
L19 0 S L18
L20 13 S L18 FUL

=> d l1
L1 HAS NO ANSWERS
L1 STR

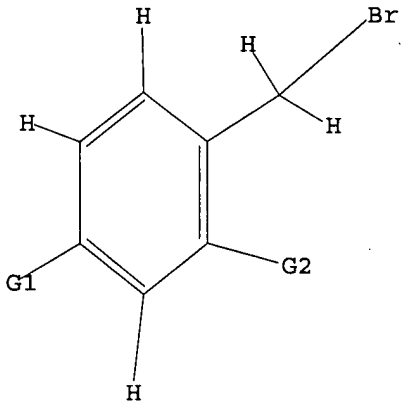


G1 Br,F

G2 H,F

Structure attributes must be viewed using STN Express query preparation.

=> d l13
L13 HAS NO ANSWERS
L13 STR



G1 Br,F

G2 H,F

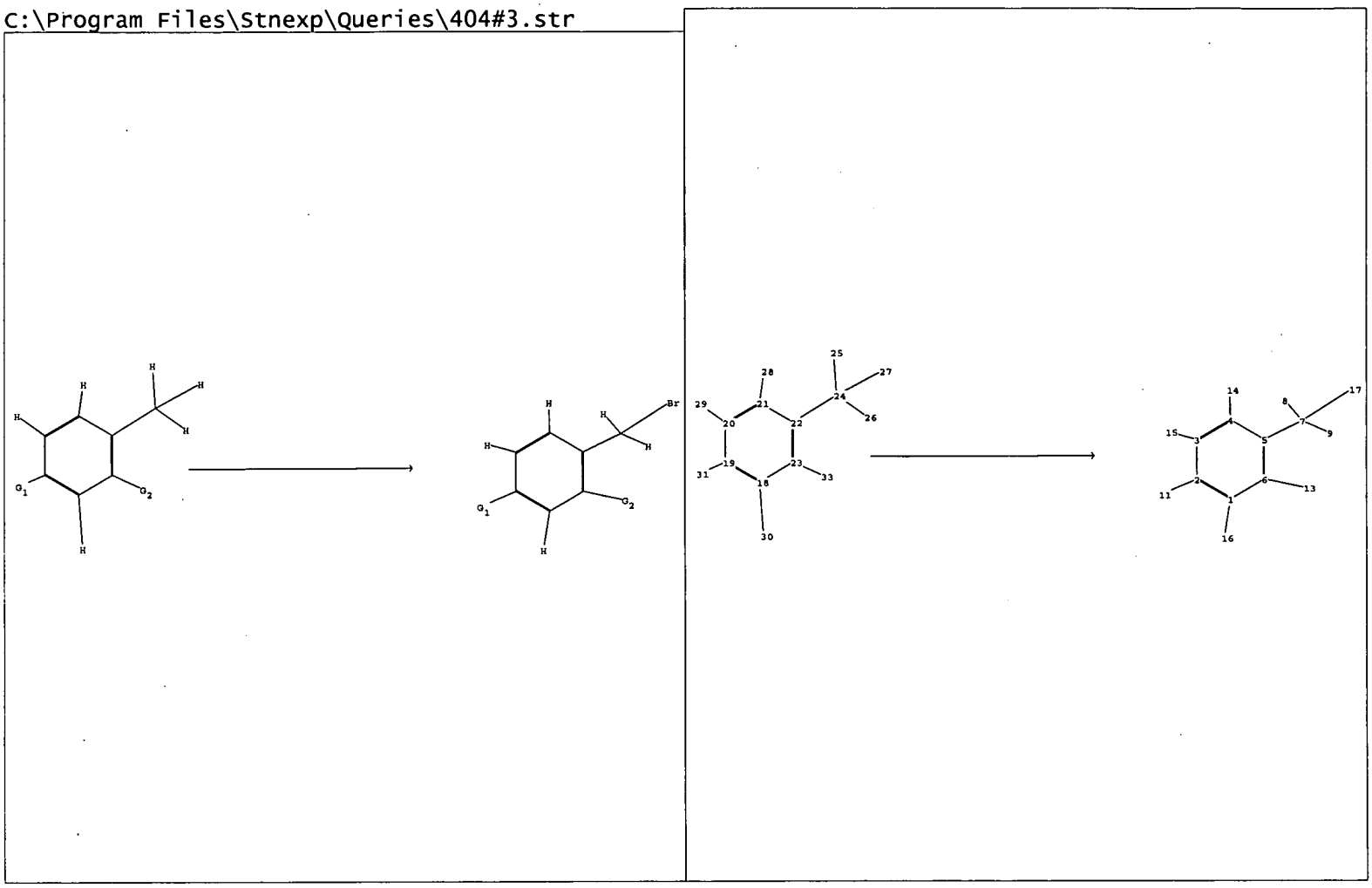
Structure attributes must be viewed using STN Express query preparation.

=> d l18
L18 HAS NO ANSWERS
L18 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

C:\Program Files\Stnexp\Queries\404#3.str



chain nodes :
7 8 9 11 13 14 15 16 17 24 25 26 27 28 29 30 31 33
ring nodes :
1 2 3 4 5 6 18 19 20 21 22 23
chain bonds :
1-16 2-11 3-15 4-14 5-7 6-13 7-8 7-9 7-17 18-30 19-31 20-29 21-28 22-24 23-33
24-25 24-26 24-27
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 18-19 18-23 19-20 20-21 21-22 22-23
exact/norm bonds :
2-11 6-13 19-31 23-33
exact bonds :
1-16 3-15 4-14 5-7 7-8 7-9 7-17 18-30 20-29 21-28 22-24 24-25 24-26 24-27
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 18-19 18-23 19-20 20-21 21-22 22-23

G1:Br,F

G2:H,F

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 11:CLASS
13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:Atom 19:Atom 20:Atom 21:Atom
22:Atom 23:Atom 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
31:CLASS 33:CLASS
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:
containing 18
reaction site bonds:
7-17:XC

L20 ANSWER 1 OF 13 CASREACT COPYRIGHT 2003 ACS on STN
AN 139:6671 CASREACT
TI Process for chemoselective thermal benzylic bromination
IN Mortensen, Max K.; Elnagar, Hassan Y.; Roy, Ranjit K.; Herndon, Robert C.; Allen, Robert H.; Caillet, David A.
PA USA
SO U.S. Pat. Appl. Publ., 7 pp.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 1

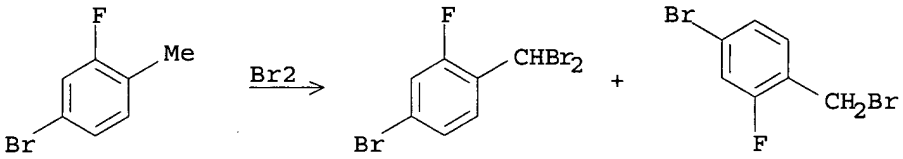
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 2003105350	A1	20030605	US 2001-10404	20011205
WO 2003055833	A1	20030710	WO 2002-US39291	20021205

W: CA, JP
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR

PRAI US 2001-10404 20011205

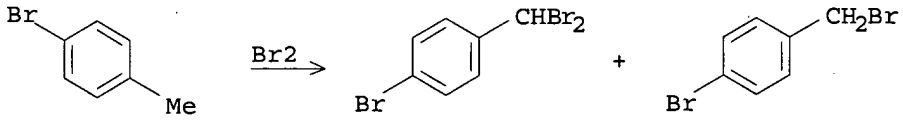
AB A thermal benzylic bromination process for producing a benzyl bromide comprises: (A) contacting gaseous bromine with a reaction mixt. having an org., liq. phase initially comprising an (un)substituted arom. ring-contg. compd. bearing one benzylic carbon atom (e.g., p-bromotoluene), the total amt. of bromine used relative to the arom. compd. being 0.2-1.2 mol of bromine per mol of arom. compd.; (B) thoroughly dispersing the gaseous bromine into the liq. phase, such that localized bromine accumulation is suppressed; and (C) maintaining the temp. of the liq. phase at 100-170.degree. so as to be sufficient to effect benzylic bromination of said the benzylic Me group (e.g., producing p-bromobenyl bromide and p-bromobenzal bromide).

RX(1) OF 2



REF: U.S. Pat. Appl. Publ., 2003105350, 05 Jun 2003
NOTE: gas phase, thermal, no solvent, chemoselective

RX(2) OF 2



REF: U.S. Pat. Appl. Publ., 7 pp.; 2003
NOTE: gas phase, alternative prepns. shown, thermal, no solvent, chemoselective

L20 ANSWER 2 OF 13 CASREACT COPYRIGHT 2003 ACS on STN
AN 133:252150 CASREACT
TI Preparation of 4-bromo-2-fluorobenzyl bromide
IN Yaginuma, Yutaka; Sugisaki, Toru; Maruta, Hiroaki; Ohashi, Masao
PA Seimi Chemical Co., Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF

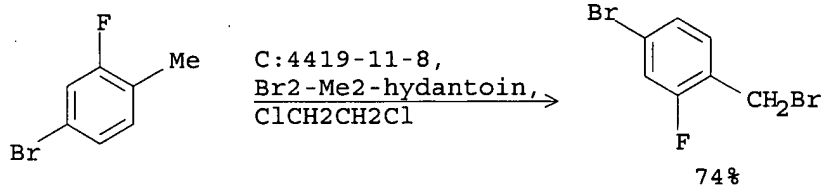
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 2000281600	A2	20001010	JP 1999-86715	19990329

PRAI JP 1999-86715 19990329

AB The title compd. (I) is prepd. by reaction of 4-bromo-2-fluorotoluene (II) with 1,3-dibromo-5,5-dimethylhydantoin (III) in the presence of radical initiators. Thus, reaction of II with III in ClCH2CH2Cl in the presence of azobis(2,4-dimethylvaleronitrile) gave 74.8% I.

RX(1) OF 1



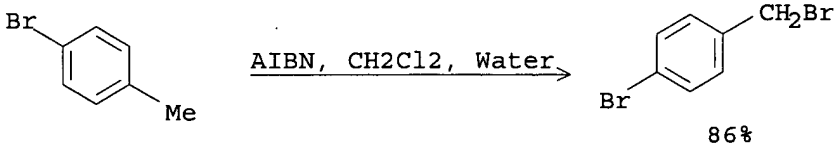
REF: Jpn. Kokai Tokkyo Koho, 2000281600, 10 Oct 2000

L20 ANSWER 3 OF 13 CASREACT COPYRIGHT 2003 ACS on STN
AN 130:352075 CASREACT
TI Preparation of electron-withdrawing group-substituted (monobromomethyl)benzenes from their corresponding methylbenzenes
IN Awano, Hiroshi; Shimoda, Atsushi; Kubo, Masashige
PA Tosoh Corp., Japan
SO Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 11130708	A2	19990518	JP 1997-298295	19971030

PRAI JP 1997-298295 19971030
OS MARPAT 130:352075
AB In .alpha.-bromination of RC6H4Me (R = NO2, halo, CF3, cyano, CO2H, alkoxycarbonyl, PhO), radical initiators chosen from dialkyl peroxides, diacyl peroxides, and azo compds. are used as catalysts in the presence of H2O. P-bromotoluene was brominated in the presence of AIBN at 35.degree. for 17 h in CH2Cl2-H2O mixt. to give 86.2% p-bromobenzyl bromide.

RX(1) OF 1

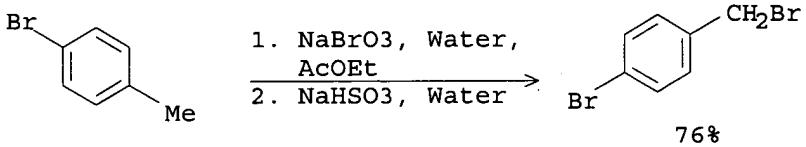


REF: Jpn. Kokai Tokkyo Koho, 11130708, 18 May 1999, Heisei

L20 ANSWER 4 OF 13 CASREACT COPYRIGHT 2003 ACS on STN
AN 129:230486 CASREACT
TI An Alternative Method for the Selective Bromination of Alkylbenzenes Using NaBrO3/NaHSO3 Reagent
AU Kikuchi, Daisuke; Sakaguchi, Satoshi; Ishii, Yasutaka

CS Department of Applied Chemistry Faculty of Engineering, Kansai University, Suita, Osaka, 564-8680, Japan
SO Journal of Organic Chemistry (1998), 63(17), 6023-6026
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
AB The chemoselective bromination of alkylbenzene derivs. was achieved using a sodium bromate/sodium hydrogen sulfite reagent.

RX(4) OF 20



76%

REF: Journal of Organic Chemistry, 63(17), 6023-6026; 1998
NOTE: chemoselective

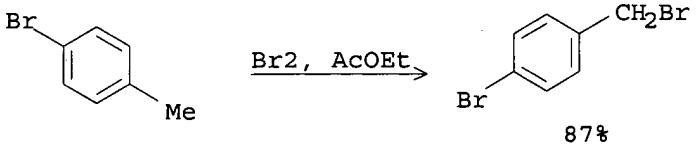
RE.CNT 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 5 OF 13 CASREACT COPYRIGHT 2003 ACS on STN
AN 129:95310 CASREACT
TI Preparation of aromatic monobromomethyl compounds
IN Kageyama, Hideki
PA Nippon Synthetic Chemical Industry Co., Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 10175883	A2	19980630	JP 1996-352745	19961212

PRAI JP 1996-352745 19961212
AB Title compds. are prepd. by bromination of benzyl position of arom. compds. with Br in ester contg. CH adjacent to CO group and/or ketone solvents. 4-BrC6H4Me was brominated with Br in AcOEt under reflux and irradn. of incandescent light for 4 h to give 87% 4-BrC6H4CH2Br.

RX(1) OF 2



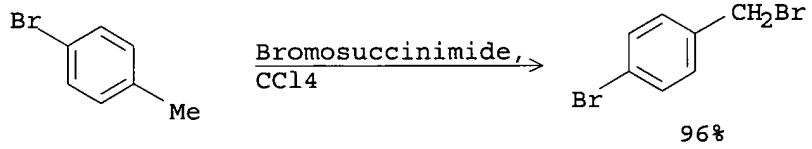
87%

REF: Jpn. Kokai Tokkyo Koho, 10175883, 30 Jun 1998, Heisei
NOTE: photochem.

L20 ANSWER 6 OF 13 CASREACT COPYRIGHT 2003 ACS on STN
AN 126:30976 CASREACT
TI The spin-delocalization substituent parameter .sigma.JJ.bul.. Part 10. The spin-delocalizing abilities of the para-trifluorovinyl and para-acetoxy groups. Synthesis of para-trifluorovinyl-, para-vinyl- and para-acetoxy-.alpha.,.beta.,.beta.-trifluorostyrenes
AU Jiang, Xi-Kui; Ji, Guo-Zhen; Wang, Daniel Ze-Rong

CS Shanghai Institute of Organic Chemistry, 354 Feng-Lin Lu, Shanghai, 200032, Peop. Rep. China
SO Journal of Fluorine Chemistry (1996), 79(2), 173-178
CODEN: JFLCAR; ISSN: 0022-1139
PB Elsevier
DT Journal
LA English
AB para-Trifluorovinyl .alpha.,.beta.,.beta.-trifluorostyrene (1-CF:CF2), p-acetoxy .alpha.,.beta.,.beta.-trifluorostyrene (1-AcO) and p-vinyl .alpha.,.beta.,.beta.-trifluorostyrene (1-CH:CH2) have been synthesized. The rate consts. (k) for the thermal cyclodimerization of 1-CF:CF2 and 1-AcO have been measured over the temp. range 90-130 .degree.C for 1-CF:CF2 and 110-160 .degree.C for 1-AcO. The .vsigma. mb polar substituent consts. of the p-CF:CF2, p-CH:CH2 and p-AcO groups calcd. from the 19F NMR chem. shifts are: for p-CF:CF2, 0.40; for p-CH:CH2, 0.03; and for p-AcO, -0.14, and the .vsigma.JJ.bul. spin-delocalization substituent consts. of the p-CF:CF2 and p-AcO groups are 0.86 and 0.35, resp., i.e., the former is a highly effective spin-stabilizer while the latter is moderately effective. Owing to the occurrence of a small amt. of side-reaction, the .vsigma.JJ.bul. value of the p-CH:CH2 group could not be accurately measured, but it was very roughly estd. to be in the range of 0.50-0.66.

RX(2) OF 14

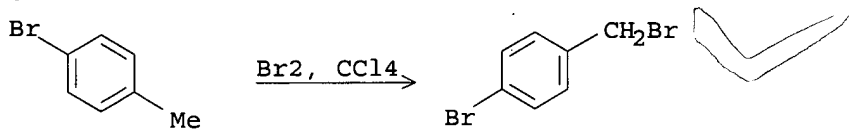


96%

REF: Journal of Fluorine Chemistry, 79(2), 173-178; 1996

L20 ANSWER 7 OF 13 CASREACT COPYRIGHT 2003 ACS on STN
AN 111:57976 CASREACT
TI Effect of structure factors on the rate of bimolecular homolytic substitution at carbon in benzylcobalt complexes
AU Dneprovskii, A. S.; Kostochkin, A. N.; Kondakov, D. Yu.
CS Leningr. Gos. Univ., Leningrad, USSR
SO Zhurnal Organicheskoi Khimii (1988), 24(5), 923-9
CODEN: ZORKAE; ISSN: 0514-7492
DT Journal
LA Russian
AB Treating RC6H4CH2Co(L)2PyH (R = H, 3- and 4-Me, 3- and 4-Br, 3- and 4-O2N; L = dimethylglyoxime monoanion; PyH = pyridine) with BrCCl3 in CHCl3 gives primarily RC6H4CH2CCl3 (same R) via a bimol. homolytic substitution reaction; the corresponding RC6H4CH2Br are also formed. The rate of substitution increases with the increase in electron-donating properties of the substituents on the arom. ring. Equimol. amts. of added pyridine or imidazole show practically no effect on the rate of reaction.

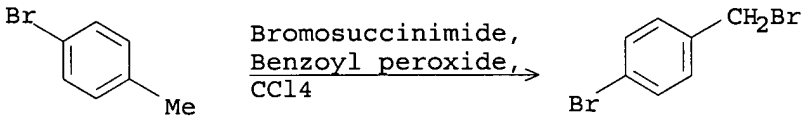
RX(13) OF 29



REF: Zhurnal Organicheskoi Khimii, 24(5), 923-9; 1988

L20 ANSWER 8 OF 13 CASREACT COPYRIGHT 2003 ACS on STN
AN 102:149497 CASREACT
TI Isolation and characterization of reactive intermediates and active catalysts in homogeneous catalysis
AU Gassman, Paul G.; Macomber, David W.; Willging, Stephen M.
CS Dep. Chem., Univ. Minnesota, Minneapolis, MN, 55455, USA
SO Journal of the American Chemical Society (1985), 107(8), 2380-8
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
AB A new method has been developed for the isolation and characterization of highly reactive intermediates and of active catalysts in homogeneous catalysis by transition-metal complexes. Using the principles of steric exclusion type chromatog., a method has been devised for the isolation of highly reactive intermediates on the surface of porous polymer films. Anal. of these surface-isolated intermediates by XPS (ESCA) provided detailed information about the transition-metal complexes that resided on the surface of the polymer film. The utility of this process was demonstrated by a reanal. of the decarbonylation of acid chlorides using chlorotris(triphenylphosphine)rhodium(I) (Wilkinson's catalyst). Through the utilization of the concepts and techniques described above, the active catalytic intermediate involved in the metathesis-promoted polymn. of cyclopentene to polypentenomer by oxotetrachlorotungsten-ethylaluminum dichloride was isolated on the surface of porous polystyrene film. This technique was viable because the active catalyst had to be attached to the end of the growing polymer chain. Anal. of the surface-isolated catalyst by XPS showed a ratio of W:O:Al:Cl of 1:1:1:4-5. The tungsten showed a binding energy of 36.0 and 38.2 eV [W(4f7/2) and W(4f5/2), resp]. This intermediate species was very labile. On treatment with trimethylphosphine, this catalyst was converted into a new tungsten complex (noncatalytic) that showed binding energies of 34.0 and 36.2 eV for W(4f7/2) and W(45/2), resp. These values can be compared to values of 34.1 and 36.3 eV for Schrock's stable tungsten-alkylidene complex, W(O)(CHCMe3)Cl2(PEt3)2.

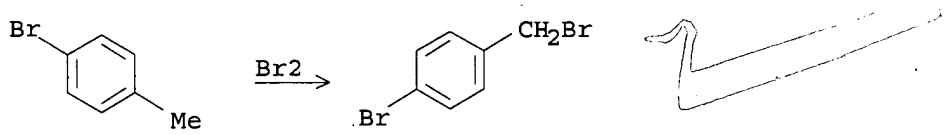
RX(15) OF 64



REF: Journal of the American Chemical Society, 107(8), 2380-8; 1985

L20 ANSWER 9 OF 13 CASREACT COPYRIGHT 2003 ACS on STN
AN 100:138318 CASREACT
TI Effect of the 1-adamantyl substituent on homolytic bromination of toluenes substituted in the ring
AU Rakhimov, A. I.; Ozerov, A. A.; Litinskii, A. O.
CS Volgogr. Politekh. Inst., Volgograd, USSR
SO Zhurnal Organicheskoi Khimii (1983), 19(12), 2630
CODEN: ZORKAE; ISSN: 0514-7492
DT Journal
LA Russian
AB The relative rate consts. for bromination of 4-RC6H4R1 (I; R = 1-adamantyl; R1 = Me, CH2Br, CHBr2) with respect to I (R = H; same R1) were 3.29, 2.24, and 1.77, resp. These values were too high to fit an LFER with .sigma.+, which was obeyed by several other I (R .noteq. 1-adamantyl).

RX(6) OF 42

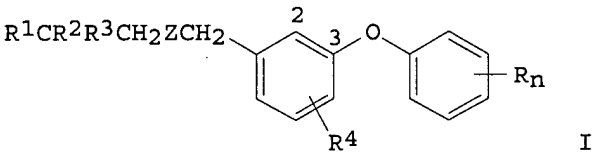


REF: Zhurnal Organicheskoi Khimii, 19(12), 2630; 1983

L20 ANSWER 10 OF 13 CASREACT COPYRIGHT 2003 ACS on STN
AN 97:181952 CASREACT
TI 2-Arylethyl ethers and sulfides as insecticides and acaricides
IN Nakatani, Kiyoshi; Numata, Satoshi; Inoue, Tsuneo; Hosono, Akira; Oda, Kengo; Kubota, Yutaka; Tachibana, Hajime; Udagawa, Takatoshi; Gohbara, Masatoshi
PA Mitsui Toatsu Chemicals, Inc. , Japan
SO Fr. Demande, 96 pp.
CODEN: FRXXBL
DT Patent
LA French
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	FR 2491924	A1	19820416	FR 1981-18848	19811007
	FR 2491924	B1	19840316		
	JP 57064632	A2	19820419	JP 1980-140600	19801009
	JP 63055500	B4	19881102		
	AU 8175549	A1	19820422	AU 1981-75549	19810922
	AU 534931	B2	19840223		
	IN 155418	A	19850126	IN 1981-CA1111	19811003
	GB 2085006	A	19820421	GB 1981-30242	19811007
	GB 2085006	B2	19850411		
	CH 649523	A	19850531	CH 1981-6439	19811007
	NL 8104586	A	19820503	NL 1981-4586	19811008
	NL 190984	B	19940701		
	NL 190984	C	19941201		
	DE 3139976	A1	19820603	DE 1981-3139976	19811008
	DE 3139976	C2	19900315		
	BR 8106509	A	19820629	BR 1981-6509	19811008
	HU 30339	O	19840328	HU 1981-2912	19811008
	HU 190521	B	19860929		
	CA 1210407	A1	19860826	CA 1981-387674	19811009
	US 4599362	A	19860708	US 1983-552871	19831118
PRAI	JP 1980-140600	19801009			
	US 1981-304964	19810923			

GI

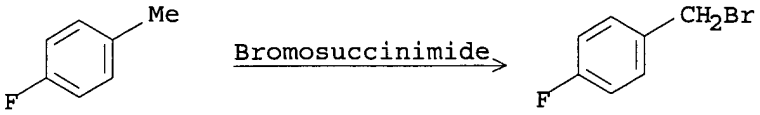


I

AB Title compds. (I; n = 1, 2; R = H, halo, alkyl, alkoxy; R1 = aryl; R2 = halo, Me, OMe; R3 = H, Me, Et; Z = O, S; R4 = halo, Me, OMe) were prepd.; they exhibit insecticidal activity and are useful as acaricides (no data). Thus, 4-ClC6H4CMe2CH2OH was treated with NaH and 3-(4-bromophenoxy)-4-fluorobenzyl bromide to give I (Rn = 4-Br, R1 = 4-ClC6H4, R2 = R3 = Me, Z

= O, R4 = 4-F).

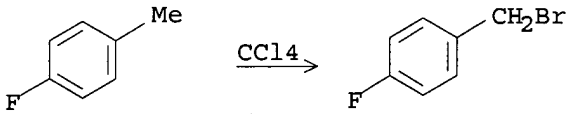
RX(8) OF 37



REF: Fr. Demande, 2491924, 16 Apr 1982

L20 ANSWER 11 OF 13 CASREACT COPYRIGHT 2003 ACS on STN
AN 52:6440 CASREACT
TI p-Fluorotropic acid and p-fluoroatropine
AU Berger, R. S.; Jacobson, A. E.; Kondritzer, A. A.
CS Army Chem. Center, MD
SO Journal of Organic Chemistry (1957), 22, 451-2
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA Unavailable
AB The prepn. of p-fluoroatropine (I) through a series of reactions starting with p-FC6H4Me (II) is reported. There are no previous reports of atropine modified by substituents on the aromatic ring. II (11 g.) refluxed 2 hrs. in 10 ml. CCl4 with 15 g. N-bromosuccinimide and the filtrate distd. gave 12.8 g. p-FC6H4CH2Br (III), b27 92-102.degree., nD 1.547. KCN (6.5 g.) in 12 ml. H2O refluxed 3 hrs. with 11.9 g. III in 30 ml. 95% alc. gave 5.3 g. p-FC6H4CH2CN (IV), b25 120-9.degree. nD 1.499. IV gave the corresponding p-FC6H4CH2CO2H (V). V (3.3 g.) in 50 ml. C6H6 refluxed 3.5 hrs. with iso-PrMgCl (from 4.2 g. iso-PrCl and 1.2 g. Mg) in Et2O, gaseous HCHO passed into the cooled mixt. from 1.72 g. paraformaldehyde heated at 180-200.degree., stirring continued 0.5 hr., and the complex hydrolyzed by pouring onto 100 ml. ice and 7 ml. concd. H2SO4 gave 2.56 g. p-fluorotropic acid (VI), m. 99.5-100.degree. (C6H6). Tropine, m. 63-4.5.degree., in Et2O treated with dry HBr gave the HBr salt (VII), decomp. 235-60.degree., for use in the esterification of VI. VI (0.74 g.) mixed with 2 ml. AcCl and, after the initial heating, heated 20 min. at 90-5.degree., the excess AcCl removed, the mixt. heated 1.5 hrs. at 90-5.degree. with 4 ml. SOCl2, the excess SOCl2 removed, and the mixt. heated 1 hr. with 0.80 g. VII, then 1 hr. with a drop of concd. HCl and 2 ml. H2O, and the product isolated gave 0.29 g. I, m. 94-5.degree. (CHCl3-ligroine); picrate, m. 181-3.degree.. The yield of I dropped to zero when the reaction temp. was lowered 20.degree.. I tested in rats for activity against Sarin showed therapeutic activity approx. the same as that of atropine.

RX(1) OF 1

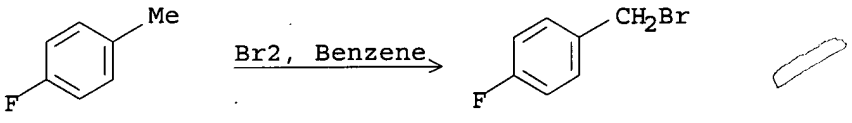


REF: Journal of Organic Chemistry, 22,, 451-2; 1957
NOTE: Classification: Bromination; # Conditions: NBS; CCl4; Rf 2h; 77 deg

L20 ANSWER 12 OF 13 CASREACT COPYRIGHT 2003 ACS on STN
AN 43:31736 CASREACT
TI Antihistamine agents. IV. Halogenated N,N-dimethyl-N'-benzyl-N'-2-pyridylethylenediamines

AU Vaughan, J. R., Jr.; Anderson, G. W.; Clapp, R. C.; Clark, J. H.; English, J. P.; Howard, K. L.; Marson, H. W.; Sutherland, L. H.; Denton, J. J.
SO Journal of Organic Chemistry (1949), 14, 228-34
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA Unavailable
AB Condensation of N,N-dimethyl-N'-2-pyridylethylenediamine with the appropriate halogenated benzyl halide in the presence of an alkali amide or hydride gave 40-60% yields of the following N,N-dimethyl-N'-2-pyridylethylenediamines: N'-4-fluorobenzyl, b0.25 130-45.degree., nD23 1.5635, m. 52-3.degree. (mono-HCl salt, m. 169.5-70.5.degree.); N'-4-chlorobenzyl (I), b1.5 178-85.degree. (mono-HCl salt, m. 172-3.6.degree.); N'-2-chlorobenzyl, b1 161-4.degree. (mono-HCl salt, m. 203-4.5.degree.); N'-4-bromobenzyl, b0.5-1.0 184-90.degree. (mono-HCl salt, m. 184-6.degree.); N'-3-bromobenzyl (II), b1 176-8.degree. (mono-HCl salt, m. 169-70.degree.); N'-4-iodobenzyl, b1 194-207.degree., nD25 1.6144 (mono-HCl salt, m.200-2.degree.). Direct bromination of N,N-dimethyl-N'-benzyl-N'-2-pyridylethylenediamine yielded N,N-dimethyl-N'-benzyl-N'-(5-bromo-2-pyridyl) ethylenediamine (mono-HCl salt, m. 180-2.degree.). An alternative synthesis of this compd. from N,N-dimethyl-N'-(5-bromo-2-pyridyl)-ethylenediamine and PhCH2Cl proved the orientation of the substituent. Direct bromination of II gave N,N-dimethyl-N'-3-bromobenzyl-N'-(5-bromo-2-pyridyl) ethylenediamine (mono-HCl salt, m. 146.5-7.5.degree.). N,N-Dimethyl-N'-benzyl-N'-(5-chloro-2-pyridyl) ethylenediamine (mono-HCl salt, m. 179-80.degree.) was obtained from 5-chloro-2-benzyl-aminopyridine (III) and Me2NCH2CH2Cl, using LiNH2. III was prepd. by refluxing 2-amino-5-chloropyridine, anhyd. HCO2H, and redistd. BzH 16 hrs., pouring into 50% NaOH and ice, and drying the solid product, m. 114-15.2.degree.. When the Li deriv. of 2-(4-chlorobenzyl-amino) pyridine (obtained from 2-aminopyridine, 4-ClC6H4CHO, and HCO2H) was treated with Me2NCH2CH2Cl, none of the desired compd. was isolated. p-ClC6H4CH2NHCH2CH2NMe2 heated with 2-bromopyridine in quinoline gave I. On comparison with pyribenzamine (IV) those derivs. halogenated in the 4-position of the benzyl group showed the highest antihistamine activity, which increased as the electronegativity of the substituent increased and the at. wt. decreased from iodo to F. The 4-bromobenzyl deriv. had approx. the same activity as IV, the 4-F deriv. was 3-4 times as active. N,N-Dimethyl-N'-2-pyridylethylenediamine with 1-C10H7CH2Cl and C6H13Br gave, resp., N,N-dimethyl-N'-1-naphthylmethyl-N'-2-pyridylethylenediamine, b1 200.degree., m. 95.degree. (mono-HCl salt, m. 224-6.degree.), and N,N-dimethyl-N'-hexyl-N'-2-pyridylethylenediamine, b1 136-46.degree., nD31.5 1.5090 (mono-HCl salt, m. 104-5.degree.). Reaction of 2-benzylaminopyridine with ClCH2COCl, followed by reaction with Et2NH and Me2NH, resp., gave N-benzyl-N-2-pyridyl-.alpha.-diethylaminoacetamide-HCl, m. 147-8.5.degree., and N-benzyl-N-2-pyridyl-.alpha.-dimethylaminoacetamide-HCl, m. 181-4.degree., in low yield. The last 4 compds. were inactive as antihistamine agents in vitro.

RX(1) OF 2

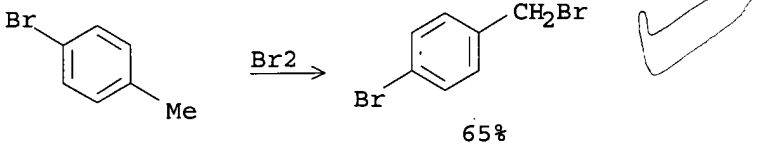


REF: Journal of Organic Chemistry, 14,, 228-34; 1949
NOTE: Classification: Bromination; # Conditions: Br2; benzene; hv

L20 ANSWER 13 OF 13 CASREACT COPYRIGHT 2003 ACS on STN
AN 40:8310 CASREACT
TI p-Bromobenzyl bromide
AU Weizmann, M.; Patai, S.

CS Hebrew Univ., Jerusalem
SO Journal of the American Chemical Society (1946), 68, 150-1
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA Unavailable
AB p-BrC6H4Me (102 g.), heated to 120.degree. in a Pyrex flask and exposed to the light of a 100-w. lamp, treated with 102 g. Br during 3 hrs. with const. agitation, gives 66% p-BrC6H4CH2Br.

RX(1) OF 1



65%

REF: Journal of the American Chemical Society, 68,, 150-1; 1946
NOTE: Classification: Bromination; # Conditions: Br2; hv; 120 deg; 3h